Synthesis and Crystal Structure of $Nb_{0.84}N$

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Z. Naturforsch. **2011**, *66b,* 1 – 6; received August 11, 2010

A new compound of the composition $Nb_{0.84}N$ was prepared by ammonolysis of NbO_2 at 1100 °C. The crystal structure refinement was performed by the Rietveld method using X-ray and neutron powder diffraction data. $Nb_{0.84}N$ crystallizes in the trigonal space group $R\bar{3}m$ (no. 166) with the lattice parameters a = 298.5(2) and c = 2384.3(4) pm. The niobium atoms form a close packing with a layer sequence which can be described by the Jagodzinski symbol *hhc*. The nitrogen atoms fill all octahedral voids. Along [001] a sequence of two layers of trigonal NbN_6 prisms and one layer of NbN_6 octahedra is formed. The nitrogen positions are fully occupied, the niobium positions only partially. $Nb_{0.84}N$ is part of a family of crystal structures between the *anti*-NiAs and the NaCl type consisting of close-packed metal layers with varying stacking sequences.

Key words: Niobium Nitride, Synthesis, Neutron Powder Diffraction, Close Packing